

APPENDIX 1 KEY DATA SUMMARY

1 CHEMICAL IDENTIFICATION

List of ALL potential by-products produced in ballast water			
Chemical Name	CAS Number	Highest Concentration (mg/L)	(bio)degradation rate or half-life (day) in Water
ACTIVE SUBSTANCES			
Hypochlorous acid ^a	7790-92-3		Decays within seconds to hours, no rate specified
Hypobromous acid ^a	13517-11-8		Decays within seconds to hours, no rate specified
RELEVANT CHEMICALS			
Bromate	15541-45-4	0.0323	15
Halogenated organic compounds			
Dichloromethane	75-09-2	0.00218	38
Bromochloromethane	74-97-5	0.01323	15
Trichloromethane	67-66-3	0.0402	38
1,2-Dichloroethane	107-06-2	0.2358	38
1,2-Dichloropropane	78-87-5	0.02978	38
Dichlorobromomethane	75-27-4	0.0157	38
Dibromochloromethane	124-48-1	0.05751	38
Tribromomethane	75-25-2	0.21692	38
Bromobenzene	108-86-1	0.08961	
Halogenated acetonitriles (HANs)			
Chloropicrin	76-06-2	0.00003	60
Bromochloroacetonitrile	83463-62-1	0.00019	38
Dibromoacetonitrile	3252-43-5	0.00525	38
Halogenated acetic acids (HAAs)			
Monobromoacetic acid	79-08-3	0.38128	8.7
Dichloroacetic acid	79-43-6	0.00465	15
Dalapon	75-99-0	0.00949	38
Trichloroacetic acid	76-03-9	0.13856	38
Bromochloroacetic acid	5589-96-8	0.079	15
Dibromoacetic acid	631-64-1	0.03043	15
Bromodichloroacetic acid	71133-14-7	0.00098	38
Tribromoacetic acid	75-96-7	0.0615	15
OTHERS CHEMICALS			
Sodium thiosulfate	7772-98-7		15
Hydrogen (%)	1333-74-0	62.4	15

^aRefer to MEPC(60/2/9).

1.1 GHS Classification

CHEMICAL NAME	PHYSICAL HAZARDS (16 HAZARD CLASSES)	HEALTH HAZARDS (10 HAZARD CLASSES)	ENVIRONMENTAL HAZARDS (1 HAZARD CLASS)
ACTIVE SUBSTANCES			
Hypochlorous acid	Corrosive to metals: Category 1		
Hypobromous acid	Cannot found		
RELEVANT CHEMICALS			
Bromate	Cannot found		
Halogenated organic compounds			
Dichloromethane	Cannot found		
Dichlorobromomethane	Cannot found		
Bromochloromethane		Skin corrosion/irritation : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (narcotic effects)	
Trichloromethane	Corrosive to metals : Category 6.1	Acute Toxicity : Category 4 Skin corrosion/irritation: Category 2 Carcinogenicity : Category 2	
1,2-dichloroethane	Pyrophoric liquids: Category 2	Acute Toxicity (oral) : Category 4 Acute Toxicity(inhalation) : Category 3 Skin corrosion/irritation : Category 2 Germ cell mutagenicity : Category 2 Carcinogenicity : Category 1B Specific target organs/systemic toxicity following single exposure : Category 1, Category 3 (narcotic effects) Specific target organs/systemic toxicity following repeated exposure : Category 1 Aspiration hazard : Category 1	
1,2-Dichloropropane	Pyrophoric liquids: Category 2	Acute Toxicity (oral): Category 4	Aquatic Toxicity:

		<p>Acute Toxicity (inhalation): Category 4</p> <p>Skin Sensitization : Category 1</p> <p>Serious eye damage / eye irritation : Category 2</p> <p>Toxic to reproduction : Category 2</p> <p>Specific target organs/systemic toxicity following single exposure : Category 1, Category 3 (narcotic effects, respiratory organs)</p> <p>Specific target organs/systemic toxicity following repeated exposure : Category 1</p>	1.Chronic 3
Dichlorobromomethane		<p>Acute Toxicity : Category 3</p> <p>Carcinogenicity : Category 1B</p> <p>Target Organ Toxicity (Repeated) : Category 2</p>	
Dibromochloromethane	Pyrophoric liquids: Category 2	<p>Acute Toxicity : Category 4</p> <p>Skin corrosion/irritation : Category 2</p> <p>Serious eye damage / eye irritation : Category 2</p> <p>Specific target organs/systemic toxicity following single exposure : Category 3 (respiratory organs), Category 3 (narcotic effects)</p> <p>Specific target organs/systemic toxicity following repeated exposure : Category 2</p>	
Tribromomethane	Corrosive to metals : Category 6.1	<p>Acute Toxicity (oral) : Category 4</p> <p>Skin corrosion / irritation : Category 2</p> <p>Serious eye damage / eye irritation : Category 2A</p> <p>Germ cell mutagenicity : Category 2</p> <p>Carcinogenicity : Category 2</p> <p>Toxic to reproduction : Category 2</p> <p>Specific target organs/systemic toxicity following single exposure : Category 1 (liver, nervous system, respiratory organs), Category 3 (narcotic effects)</p> <p>Specific target organs/systemic toxicity following repeated exposure : Category 1 (liver), Category 2 (kidneys, thyroid gland, nervous system)</p>	

Bromobenzene	Pyrophoric liquids: Category 2	Skin corrosion / irritation : Category 2 Serious eye damage / eye irritation : Category 2 Specific target organs/systemic toxicity following single exposure : Category 2 Specific target organs/systemic toxicity following repeated exposure : Category 2 Aspiration hazard : Category 2	Aquatic Toxicity: 1.Chronic 2
<i>Halogenated acetonitriles (HANs)</i>			
Chloropicrin		Acute Toxicity (oral) : Category 3 Acute Toxicity (inhalation) : Category 1 Skin corrosion/irritation : Category 2 Serious eye damage / eye irritation : Category 1 Specific target organs/systemic toxicity following single exposure : Category 1, Specific target organs/systemic toxicity following repeated exposure : Category 1	Aquatic Toxicity: 1.Acute 1 2.Chronic 1
Bromochloroacetonitrile	Cannot found		
Dibromoacetonitrile		Acute Toxicity (oral) : Category 3 Acute Toxicity (dermal) : Category 4 Acute Toxicity (Inhalation) : Category 4	
<i>Halogenated acetic acids (HAAs)</i>			
Monobromoacetic acid		Acute Toxicity (oral) : Category 2 Acute Toxicity (Dermal) : Category 2 Skin corrosion / irritation : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (respiratory organs)	
Dichloroacetic acid	Corrosive to metals : Category 1	Acute Toxicity (Dermal) : Category 3 Skin corrosion / irritation : Category 2 Serious eye damage / eye irritation : Category 1 Germ cell mutagenicity : Category 2 Carcinogenicity : Category 2	
Dalapon		Skin corrosion / irritation : Category 2	

Trichloroacetic acid		Skin corrosion / irritation : Category 1 Serious eye damage / eye irritation : Category 1 Germ cell mutagenicity : Category 2 Carcinogenicity : Category 2 Toxic to reproduction : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (narcotic effects) Specific target organs/systemic toxicity following repeated exposure : Category 2	
Bromochloroacetic acid	Cannot found		
Dibromoacetic acid		Acute Toxicity (inhalation) : Category 1B Skin contact, ingestion and skin corrosion : Category 1B	
Bromodichloroacetic acid	Cannot found		
Tribromoacetic acid		Acute Toxicity : Category 2	
<i>OTHERS CHEMICALS</i>			
Sodium thiosulfate		Skin corrosion/irritation : Category 2 Serious eye damage / eye irritation : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (respiratory organs) Specific target organs/systemic toxicity following repeated exposure : Category 2	
Hydrogen	Flammable gases : Category 1 Gases under pressure		

2 Data on each component of the preparation and by-producted in ballast water

A detail information refer to Appendix 5 MSDS. In this dossier, monobromoacetic acid and trichloroacetic acid of RCs are described.

2 EFFECTS ON AQUATIC ORGANISMS OF MONOBROMOACETIC ACID

2.1 Acute Aquatic Toxicity Data - N/A

2.2 Chronic Aquatic Toxicity Data on WET

	Species	LC50 (mg/l/duration)	Reference
Fish	N/A		
Crustacea	<i>Daphnia magna</i>	1.6/21 d	ECOTOX : aquatic report, 2011
Algae	N/A		

2.3 Information on Endocrine Disruption - N/A

2.4 Sediment Toxicity - N/A

2.5 Bioavailability/Biomagnification/Bioconcentration

	Measured/Calculated	Reference
Log Pow	0.43 (KOWWIN v. 1.67)	EPI Suite, 2011
BCF	3.162 L/kg wet-wt (regression-based estimate)	
	1.102 L/kg wet-wt (Arnot-Gobas Method)	

2.6 Food Web/Population Effects - N/A

3 MAMMALIAN TOXICITY OF MONOBROMOACETIC ACID

3.1 Acute mammalian Toxicity

	Value	Species	Reference
Oral LD ₅₀ (mg/l)	177 mg/kg	Rat	WHO, 2004b HSDB, 2011
Dermal LD ₅₀ (mg/l)	N/A		
Inhalation LC ₅₀ (mg/l/4h)	N/A		

3.2 Corrosion/Irritation - N/A

3.3 Sensitization- N/A

3.4 Repeated-Dose Toxicity

Exposure Route	Oral exposure (Drinking water)
Exposure Duration	2 or 14 days
Exposure dose	0 or 100 mg/kg MBA in a volume of 5 mL/kg in water
Species	Sprague-Dawley rat
Method	
Results	The selected single dose of 100 mg/kg was an approximate LD ₀₁ , and was chosen to provide a

	relatively-high dose with a minimal likelihood of mortality. Measures of male reproductive toxicity included reproductive-organ weights, sperm counts, sperm morphology, sperm motility, and histopathological examination of the seminiferous tubules. No adverse effects were observed in the single-dose study; therefore, a repeated-dosing protocol experiment was also conducted. Groups of eight rats were given daily doses of 0 or 25 mg/kg/day MBA in water for 14 days, and were sacrificed 24 hours after the last dose. MBA also failed to induce any spermatotoxicity in this repeated-dosing study.
NOAEL	
NOEL	
Reference	U.S. EPA, 2005

3.5 Development and Reproductive Toxicity

Exposure Route	Oral intubation
Exposure Duration	Gestation days 6-15
Exposure dose	0, 25, 50 or 100 mg/kg/day
Species	Pregnant Long Evans rats
Method	
Results	In the high-dose group, maternal weight-gain was reduced and one dam died. No effects on reproduction were observed. Several developmental effects were noted in the high-dose group, including decreased size of live fetuses (the affected measure of size was not provided in the study summary) and increased incidence of soft-tissue malformations, most of which were cardiovascular and craniofacial.
NOAEL	50 mg/kg/day
LOAEL	100 mg/kg/day
NOEL	
Reference/Comments/ Justification for missing data	HSDB, 2011 U.S. EPA, 2005

3.6 Carcinogenicity/Mutagenicity/Reprotoxicity – Please include the EHS rating and that of any other recognized body

	Species	Method Details	Results	Reference
Carcinogenicity	N/A			
Mutagenicity	L-1210 mouse leukaemia cells	SOS chromotest	Negative	WHO, 2004b
Reprotoxicity	Sprague-Dawley rats	Spermatotoxicity	No adverse	

4 ENVIRONMENTAL FATE AND EFFECT UNDER AEROBIC AND ANAEROBIC CONDITIONS OF MONOBROMOACETIC ACID

4.1 Modes of Degradation (biotic and abiotic)

	Seawater or Fresh Water	Test Duration	Results	Break-down products	Reference
Hydrolysis pH 5	Monobromoacetic acid is not expected to undergo hydrolysis in the environment due to the lack of functional groups that hydrolyze under environmental conditions				HSDB, 2011
Hydrolysis pH 7					
Hydrolysis pH 9					
Biodegradation	AEROBIC: Monobromoacetic acid, present at 2 mg/L, reached 82% of its theoretical biological oxygen demand using the OECD Closed Bottle Test when using preacclimatized inoculum derived from a Zahn-Wellens test. An OECD Closed Bottle Test performed in the same study using an unacclimatized inoculum classified the compound as not readily biodegradable. Monobromoacetic acid was utilized as a carbon source by several Pseudomonas strains; growth was visible within one week.				
1/2-Life	Water		8.7 d		EPI Suite, 2011

4.2 Partition Coefficients

	Method	Results	Reference
Log Pow	KOWWIN v. 1.67	0.43	EPI Suite, 2011
Koc	KOCWIN v. 2.00	2.413	

4.3 Persistence and Identification of Main Metabolites

	Method	Results	Reference
Persistence	BIOWIN v. 1.67	3.2857	EPI Suite, 2011

4.4 Reaction with Organic Matter - N/A

4.5 Potential Physical Effects on Wildlife and Benthic Habitats - N/A

4.6 Potential Residues in Seafood - N/A

4.7 Any Known Interactive Effects - N/A

5 PHYSICAL AND CHEMICAL PROPERTIES FOR THE ACTIVE SUBSTANCES, PREPARATIONS AND TREATED BALLAST WATER, IF APPLICABLE OF MONOBROMOACETIC ACID

Property	Value	Reference
Melting point (°C)	29.19 (MPBPVP v. 1.43)	EPI Suite, 2011

Boiling point (°C)	192.67 (MPBPVP v. 1.43)	EPI Suite, 2011
Flammability (flash point for liquids; °C)	N/A	
Density (20°C; kg/m³)	1.93 g/mL	WHO, 2004b
Vapour pressure (20°C; Pa)	0.131 mm Hg at 25 °C (MPBPVP v. 1.43)	EPI Suite, 2011
Vapour density (air = 1)		
Water solubility (temp; effect of pH; mg/L)	9.379×10 ⁴ mg/L at 25 °C (WSKOW v.1.41)	EPI Suite, 2011
pH in solution		
Dissociation constant (pKa)	2.89	HSDB, 2011
Oxidation-reduction potential		
Corrosivity to material or equipment	Irritating and corrosive to skin and mucous membranes	HSDB, 2011
Reactivity to container material		
Auto-ignition temperature (°C)		
Explosive properties		
Oxidizing properties		
Surface tension		
Viscosity (mPa.s)		
Thermal stability and identity of breakdown products		
Other physical or chemical properties		

6 OTHER INFORMATION OF MONOBROMOACETIC ACID

6.1 Analytical Methods for Measuring the Concentration at environmentally Relevant Concentrations - N/A

6.2 Material Safety Data Sheet provided (Yes)

6.3 GHS Classification

PHYSICAL	HEALTH	ENVIRONMENTAL
	Acute Toxicity (oral): Category 2 Acute Toxicity (Dermal): Category 2 Skin corrosion / irritation : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (respiratory organs)	Aquatic Toxicity: 1.Acute 1

6.4 Risk Characterization (Refer to Appendix 5 Material Safety Data sheet)

Persistent (V/T) (y/n)	Bioaccumulative (B/P) (y/n)	Toxic (y/n)
3.2857/ 8.7d NO	1.102/0.43 NO	1.6 mg/L/21d (LC ₅₀ , crustacea) NO

2 EFFECTS ON AQUATIC ORGANISMS OF TRICHLOROACETIC ACID

2.1 Acute Aquatic Toxicity Data

	Species	LC50 (mg/l/duration)	Reference
Fish	<i>Salmonidae</i>	1050/4 d	ECOTOX : aquatic report, 2011
Crustacea	<i>Sterptocephalus proboscideus</i>	1.2/24 hr	
Algae	N/A		

2.2 Chronic Aquatic Toxicity Data

	Species	LC50 (mg/l/duration)	Reference
Fish	<i>Cyprinus carpio</i>	7/63 d (LOEC)	OECD SIDS, 2000
Crustacea	N/A		
Algae	<i>Chlorella pyrenoidosa</i>	0.3/14 d	IMO, 2009b

2.3 Information on Endocrine Disruption - N/A

2.4 Sediment Toxicity - Trichloroacetic acid concentration in soil ranges from 0.1 to 380 ug/kg dry soil (Schöler HF et al., 2003). General soil studies indicate that dalapon and trichloroacetic acid are subject to microbial decomposition, but that trichloroacetic acid is degraded more slowly than dalapon. It was reported that disappearance of trichloroacetic acid from soil was favored by warm, moist condition. Also it was also found that breakdown by trichloroacetic acid in solis was most rapid under conditions conducive to high microbial activity. trichloroacetic acid breakdown was low in in sandy soils (HSDB, 2011).

2.5 Bioavailability/Biomagnification/Bioconcentration

	Measured/Calculated	Reference
Log Pow	1.44 (KOWWIN v. 1.67)	EPI Suite, 2011
BCF	3.162 L/kg wet-wt (regression-based estimate)	
	3.024 L/kg wet-wt (Arnot-Gobas Method)	

2.6 Food Web/Population Effects - N/A

3 MAMMALIAN TOXICITY OF TRICHLOROACETIC ACID

3.1 Acute mammalian Toxicity

	Value	Species	Reference
Oral LD ₅₀ (mg/l)	4970 mg/kg	Mouse	OECD SIDS, 2000
Dermal LD ₅₀ (mg/l)	> 2000 mg/kg	Rats	
Inhalation LC ₅₀ (mg/l/4h)	> 4800 ppm	Rat, Rabbit, Cat, Guinea pig	

3.2 Corrosion/Irritation

	Species	Method	Results	Reference
Skin	human		Very hazardous in case of skin contact (irritant). Hazardous in case of skin contact (corrosive). Slightly hazardous in case of skin contact (permeator).	ScienceLab MSDSb
Eye	Human		Hazardous in case of eye contact (corrosive).	

3.3 Sensitization - N/A

3.4 Repeated-Dose Toxicity

Exposure Route	Oral exposure
Exposure Duration	10 weeks
Exposure dose	0 or 0.025 g/L (0 or 3.8 mg/kg/d)
Species	Rats
Method	
Results	Decreased body weight and kidney glutathione levels. Changed serum markers of lipid and carbohydrate metabolism. Mild liver and kidney histopathology.
NOAEL	
LOAEL	3.8 mg/kg/d
NOEL	
Reference	IMO, 2009b

3.5 Development and Reproductive Toxicity

Exposure Route	Oral exposure
Exposure Duration	Gestation days 1 to 22
Exposure dose	0 or 2.73 g/L (0 or 290 mg/kg/d)
Species	Rats
Method	
Results	Decreased maternal body weight gain. Increased resorption and cardiac soft tissue malformations.
NOAEL	
LOAEL	290 mg/kg/d(maternal, reproductive and developmental)
NOEL	
Reference/Comments/ Juristification for missing data	IMO, 2009b

3.6 Carcinogenicity/Mutagenicity/Reprotoxicity – Please include the EHS rating and that of any other recognized body

	Species	Method Details	Results	Reference
Carcinogenicity	Mice	Drinking water	No evidence (female) Increased incidence of tumours in the liver of the male	OECD SIDS, 2000
Mutagenicity	<i>Salmonella typhimurium</i> strain TA98, TA100	Histidine reversion	Negative	IARC, 2004b
Reprotoxicity	Swiss mice	Sperm head abnormality	Positive	IMO, 2009b

4 ENVIRONMENTAL FATE AND EFFECT UNDER AEROBIC AND ANAEROBIC CONDITIONS OF TRICHLOROACETIC ACID

4.1 Modes of Degradation (biotic and abiotic)

	Seawater or Fresh Water	Test Duration	Results	Break-down products	Reference
Hydrolysis pH 5 Hydrolysis pH 7 Hydrolysis pH 9	Hydrolysis is not expected to be an important environmental fate process since this compound lacks functional groups that hydrolyze under environmental conditions.				HSDB, 2011
Biodegradation	Activated sludge	4 weeks	7%		IMO, 2009b
	AEROBIC: Trichloroacetic acid, present at 100 mg/L, reached 7% of its theoretical BOD in four weeks using an activated sludge inoculum at 30 mg/L and the Japanese MITI test. The rate of degradation of trichloroacetic acid was studied in untreated, fertilized, and limed fine sand and humus soil. The soils were treated with 12.6 mg/kg radioactively labeled TCA and the total count of bacteria able to utilize trichloroacetic acid for growth was determined after two weeks of inoculated bacteria incubation at 14-15 °C. Bacteria able to grow in trichloroacetic acid fine sand samples ranged from about 25 to 275 CFU X 10 ⁵ /g soil; growth on trichloroacetic acid humus samples ranged from about 15 to 60 CFU X 10 ⁶ /g soil. Liming increased the rate of trichloroacetic acid degrading bacteria, especially in sandy soil. A half-life of trichloroacetic acid in soil was reported as 119.6 days in a laboratory experiment. General soil studies indicated that trichloroacetic acid was subject to microbial decomposition. Disappearance of trichloroacetic acid was favored by warm moist conditions and trichloroacetic acid breakdown in soils				HSDB, 2011

	was most rapid under conditions conducive to high microbiological activity. Trichloroacetic acid breakdown was low in sandy soils. Trichloroacetic acid experienced a lag period in biodegradation: a period in which low degradation was followed by rapid degradation.				
1/2-Life	Water		38 d		EPI Suite, 2011

4.2 Partition Coefficients

	Method	Results	Reference
Log Pow	KOWWIN v. 1.67	1.44	EPI Suite, 2011
Koc	KOCWIN v. 2.00	7.787	

4.3 Persistence and Identification of Main Metabolites

	Method	Results	Reference
Persistence	BIOWIN v. 1.67	2.4710	EPI Suite, 2011

4.4 Reaction with Organic Matter - N/A

4.5 Potential Physical Effects on Wildlife and Benthic Habitats - N/A

4.6 Potential Residues in Seafood - N/A

4.7 Any Known Interactive Effects - N/A

5 PHYSICAL AND CHEMICAL PROPERTIES FOR THE ACTIVE SUBSTANCES, PREPARATIONS AND TREATED BALLAST WATER, IF APPLICABLE OF TRICHLOROACETIC ACID

Property	Value	Reference
Melting point (°C)	26.70 (MPBPVP v. 1.43)	EPI Suite, 2011
Boiling point (°C)	203.15 (MPBPVP v. 1.43)	EPI Suite, 2011
Flammability (flash point for liquids; °C)		
Density (20°C; kg/m³)	900	OECD SIDS, 2000
Vapour pressure (20°C; Pa)	0.196 mmHg at 25 °C (MPBPVP v. 1.43)	EPI Suite, 2011
Vapour density (air = 1)	5.6	IMO, 2009b
Water solubility (temp; effect of pH; mg/L)	1.199E+004 mg/L at 25 °C	EPI Suite, 2011
pH in solution	1.2 in 0.1 M solution	HSDB, 2011
Dissociation constant (pKa)	0.7	OECD SIDS, 2000
Oxidation-reduction potential	Not available	IMO, 2009b

Corrosivity to material or equipment	Iron, zinc and aluminum Extremely corrosive to skin on prolonged contact	HSDB, 2011
Reactivity to container material		
Auto-ignition temperature (°C)		
Explosive properties		
Oxidizing properties		
Surface tension	27.8 dynes/cm (80.2 °C)	HSDB, 2011
Viscosity (mPa.s)		
Thermal stability and identity of breakdown products		
Other physical or chemical properties		

6 OTHER INFORMATION OF TRICHLOROACETIC ACID

6.1 Analytical Methods for Measuring the Concentration at environmentally Relevant Concentrations - N/A

6.2 Material Safety Data Sheet provided (Yes)

6.3 GHS Classification

PHYSICAL	HEALTH	ENVIRONMENTAL
	Skin corrosion / irritation : Category 1 Serious eye damage / eye irritation : Category 1 Germ cell mutagenicity : Category 2 Carcinogenicity: Category 2 Toxic to reproduction : Category 2 Specific target organs/systemic toxicity following single exposure : Category 3 (narcotic effects) Specific target organs/systemic toxicity following repeated exposure : Category 2	

6.4 Risk Characterization (Refer to Appendix 5 Material Safety Data sheet)

Persistent (V/T) (y/n)	Bioaccumulative (B/P) (y/n)	Toxic (y/n)
2.4710/ 38d NO	3.024/1.44 NO	0.3mg/L/14d (LC ₅₀ , algae) NO